Subject Code : ECN3BC

COMPUTATIONAL CHEMISTRY

UNIT-I

01. Introduction to computing and networking.

Introduction to computers and computing – hardware – basic organization of a computer – CPU – Main memory – secondary storage – I/O devices – software – system and application software – high and low level languages – compilers – algorithms and flow charts.

(9 Hours)

02. Introduction to networking – computer networks – network components – hubs – switches, repeaters, routers, bridges and gateways – LAN, WAN, intranet and internet – worldwide web – internet for chemists – online search of chemistry databases – e-journals – search engines for chemistry – chemweb.

(9 Hours)

UNIT-II

C Programming-I

03. Structure of a C program – data types – constants and variables**,** keywords, operators and expression

(9 Hours)

04. Control structure – if, if-else, nested if-else, while, while – do, for, nested for, goto, continue, break, switch case statements.

(9 Hours)

UNIT- III

C- Programming-II

05. Arrays – user defined functions (recursion) - call by value and call by reference – string functions – preprocessors – storage class – structure and union.

(9 Hours)

06. Pointers – pointer expressions, arithmetic passing pointers through arrays and functions – file handling – introduction to OOPS

(9 Hours)

UNIT – IV

C Programming-III Applications

07. Solution of equations – Bisection and Newton-Raphson methods – Linear simultaneous equations – Gauss elimination.Linear least square fitting. Numerical differentiation – Newton forward, backward and central difference formulae. Numerical integeration – trapezoidal rule and Simpson's method.

(For the above methods algorithms may be discussed and C programmes may be developed for chemistry examples)

(18 Hours)

UNIT – V

Molecular Modelling Basics

08. Molecular modeling – coordinate systems – cartesian and internal coordinate systems – bond lengths, bond angles and torsion angles – distance matrix – stick models – space filling models – potential energy surfaces – Molecular mechanics – application and paramererization-advantages and limitations of force fields.

(18 Hours)

Text books and References:

1. E. Balaguruswamy, "*Programming in ANSI C*", Tata McGraw Hill, 2nd Edition, New Delhi, 1999.
2. Robert Lafore**, "***Object Oriented Programming in Turbo C++***",** Galgotia, New Delhi, 1995.
3. K. V. Raman, "*Computers in Chemistry*", Tata McGraw Hill, New Delhi, 1993.
4. H. M. Antia, "*Numerical Methods for Scientists and Engineers*", Tata McGraw Hill.
5. E. Balaguruswamy, "*Fortran for Beginners*", Tata McGraw Hill, New Delhi, 1990
6. S. K. Basandra, "*Local Area Networking*", Galgotia, New Delhi, 1999.
7. A. S. Taneubaum, "*Computer Networks*", Prentice Hall of India, 1996.
8. S. M. Bachrach, "*Internet for Chemists*", ACS Publications, Washigton, DC, 1996.
9. K. B. Hipkowitz and D. B. Boyd (Ed), "*Reviews in Computational Chemistry*", VCH, New York, 1990.
10. H. RZepa, "*The Internet as a Computational Chemistry Tool*", J. Mol. Struct., (Theochem), 398-399 (1997) 27-33.
11. Christin Crumbish, "*The ABC's of the Internet* " 2nd Edition..
12. A. R. Leach, "*Molecular Modelling Principles and Applications*", 2nd Edition, Prentice Hall, 2001.
13. W. B. Smith, "*Introduction to Theoretical Organic Chemistry and Molecular Modelling*", John Wiley, New York, 1996.
14. Tim Clark, "*A Handbook of Computational Chemistry*", John Wiley, New York, 1985.